LIST OF CONTENTS

NUMBER 1

i Softstrip® data strip containing the table of contents of this issue

iii Softstrip® data strip containing the table of contents of Vol. 11, No. 6

C. A. Ruiz, I. T. Cameron and **R. Gani** — 1 A generalized dynamic model for distillation columns—III. Study of startup operations

E. F. Vogel and **T. F. Edgar** — 15 An adaptive pole placement controller for chemical processes with variable dead time

S. K. Shum, J. F. Davis, W. F. Punch III and **B. Chandrasekaran** — 27 An expert system approach to malfunction diagnosis in chemical plants

P. L. Mills, S. Lai, M. P. Duduković and **P. A. Ramachandran** — 37 A numerical study of approximation methods for solution of linear and nonlinear diffusion–reaction equations with discontinuous boundary conditions

S. Venkataraman and **A. Lucia** — 55 Solving distillation problems by Newton-like methods

J. M. Montagna and **O. A. Iribarren** — 71 Optimal computation sequence in the simulation of chemical plants

M. L. Steemson and **E. T. White** — 81 Numerical modelling of steady state continuous crystallization processes using piecewise cubic spline functions

J. R. Paloschi and **J. D. Perkins** — 91 Scale invariant quasi-Newton methods for the solution of nonlinear equations

D. J. Vickery, J. J. Ferrari and **R. Taylor** — 99 An "efficient" continuation method for the solution of difficult equilibrium stage separation process problems

J. F. Cordoba — 105 A linear algorithm for nonredundant decompositions

NUMBER 2/3

MATCHEM Issue

P. Jedlovszky — v Introductory remarks

Obtaining Data

Review Paper
D. W. T. Rippin — 109 Statistical methods for experimental planning in chemical engineering

G. Bánvölgyi, P. Valkó, S. Vajda and **N. Fülöp** 117 Estimation of influential parameters in a steady-state evaporator model: the principal component approach

L. Timár, J. Siklós and **J. Édes** 123 Computer generation of thermodynamic property charts for mixtures

K. Varga, I. Marsi, G. Tasi, I. Kiricsi and **P. Fejes** 127 Facilitation of computer estimation of kinetic parameters of a heterogeneous catalytic reaction via the use of adsorption data

K. M. Hangos and **J. Tóth** 135 Maximum likelihood estimation of reaction-rate constants

S. Wasylkiewicz and **J. Piotrowicz** 141 Deviations from ideality in weak electrolyte solutions

Sub-Unit Problems

W. Błasiak and **W. Gajewski** 147 Modelling of motion of reacting particles in two-phase systems

A. Brunovská 153 Deactivation of a catalyst pellet with nonuniform activity distribution

J. Hunek, J. Sawinsky, A. Bálint and **L. Podmaniczky** 159 Computer-aided measurement and evaluation of residence-time-distribution curves

B. Lakatos and **E. Varga** 165 Probability density functions based micromixing model of chemical reactors

Unit Operations

D. Adamska-Rutkowska, A. Stankiewicz and **Z. Leszczynski** 171 Simulation of the operational characteristics of the large-scale multitubular reactor for maleic anhydride production

B. Biscans and **J. Bertrand** 177 Modelling of a continuous flow electrophoresis cell computation procedure design

G. Halász, J. Tóth and **K. M. Hangos** 183 Energy-optimal operation conditions of a tunnel kiln

P. Glavič, Z. Kravanja and **M. Homšak** 189 Modelling of reactors for process heat integration

J. Jelínek 195 The calculation of multistage equilibrium separation problems with various specifications

P. Rosendorf, M. Kubíček and **J. Schöngut** 199 On-line optimization of a rectification column

L. Neužil, F. Procházka, V. Bejček and **M. Mocek** 205 Modelling a two-stage countercurrent fluidized bed reactor for removing SO_2 from gases by active soda

I. Zbicinski, S. Grabowski, C. Strumillo, L. Kiraly and **W. Krzanowski** 209 Mathematical modelling of spray drying

Synthesis

P. Árva and **B. Csukás** 215 Computer-aided process synthesis by fuzzy valuated structures

I. Mészáros and **Z. Fonyó** 225 Extensive state optimization for heat-integrated distillation columns

R. Ptáčník and **J. Klemeš** 231 An application of mathematical optimization methods in heat-exchange network synthesis

Process Dynamics

L. Pellegrini, G. Biardi and **M. G. Grottoli** 237 Determination of the region of asymptotic stability for a CSTR

V. M. Schevtsova and **Yu. S. Ryazantsev** 243 Numerical investigation of the multiplicity of the steady-state regimes in a tubular reactor with reaction of the Langmuir–Hinshelwood type

A. Buso, A. Paratella and **A. Trotta** 247 The solution of the dynamic adsorption beds using the finite element method

Special Topics

A. J. Czulek 253 An experimental simulator for batch chemical processes

J. M. Martinez-Benet and **L. Puigjaner** 261 A powerful improvement on the methodology for solving large-scale pipeline networks

I Softstrip® data strip containing the table of contents of this issue

NUMBER 4

i Softstrip® data strip containing the table of contents of this issue

G. E. Paules IV and **C. A. Floudas** 267 Synthesis of flexible distillation sequences for multiperiod operation

H. Galindez and **Aa. Fredenslund** 281 Simulation of multicomponent batch distillation processes

G. M. Ostrovsky, M. C. Ostrovsky and **T. A. Berezhinsky** 289 Optimization of chemical plants with recycles

M. Mulholland 297 Application of minimum-variance control strategies on an ammonia plant

Y. Arkun and **C. O. Morgan III** — 303 On the use of the structured singular value for robustness analysis of distillation column control

P. Engel and **M. Morari** — 307 Limitations of the primary loop-breaking method for synthesis of heat-exchanger networks

Y.-D. Lang, L. T. Biegler and **I. E. Grossmann** — 311 Simultaneous optimization and heat integration with process simulators

R. L. Kirkwood, M. H. Locke and **J. M. Douglas** — 329 A prototype expert system for synthesizing chemical process flowsheets

S. Prakash and **J. L. Gaddis** — 345 An exponential transformation to assist in solution of polarization boundary layers in membrane separation

Short Note

A. Bhattacharya and **B. Joseph** — 351 Simulation of fixed-bed gas–solid reactors using an adaptive-spline collocation method

355 Announcement

NUMBER 5

CEF'87 Issue

G. Buzzi-Ferraris and **S. Pierucci** — v Introduction

L. T. Biegler — 357 On the simultaneous solution and optimization of large scale engineering systems

Dominique Bonvin and **Urs Saner** — 371 On line procedures for supervising the operation of batch reactors

G. D. Byrne and **P. R. Ponzi** — 377 Differential-algebraic systems, their applications and solutions

L. Chacon-Mondragon and **D. M. Himmelblau** — 383 A new definition of flexibility for chemical process design

M. Dente, S. Pierucci, A. Sogaro, G. Carloni and **E. Rigolli** — 389 Simulation program for urea plants

J. P. Fletcher and **J. E. Ogbonda** — 401 A modular equation-oriented approach to dynamic simulation of chemical processes

M. Hillestad and **T. Hertzberg** — 407 Convergence and stability of the sequential modular approach to dynamic process simulation

H. Hofmann — 415 Future trends in chemical engineering modelling

P. Holl, W. Marquardt and **E. D. Gilles** — 421 DIVA—a powerful tool for dynamic process simulation

Jaroslav Jelínek and **Radim Ptáčník** 427 Synthesis of heat integrated rectification systems

David Juarez-Romero and **R. W. H. Sargent** 433 Improving the robustness of the moving finite element method

M. Lázaro and **L. Puigjaner** 443 Solution of integer optimization problems subjected to non-linear restrictions: an improved algorithm

C. C. Pantelides, D. Gritsis, K. R. Morison and **R. W. H. Sargent** 449 The mathematical modelling of transient systems using differential-algebraic equations

Heinz A. Preisig, Mark Kimmich and **David W. T. Rippin** 455 A study of dynamic system modelling

J. Rennotte and **B. Kalitventzeff** 461 Contribution to the thermodynamic study of electrolyte solutions

G. J. Smith and **W. Morton** 469 Dynamic simultation using an equation-orientated flowsheeting package

G. Storti, M. Masi, R. Paludetto, M. Morbidelli and **S. Carrà** 475 Adsorption separation processes: countercurrent and simulated countercurrent operations

Robert J. Topliss, Dimitrios Dimitrelis and **John M. Prausnitz** 483 Computational aspects of a non-cubic equation of state for phase-equilibrium calculations. Effect of density-dependent mixing rules

A. Vetere, O. Sguera, A. Paggini and **D. Sanfilippo** 491 Vapor–liquid equilibria applied to MAS mixtures

i Softstrip® data strip containing the table of contents of this issue

NUMBER 6

i Softstrip® data strip containing the table of contents of this issue

Review Paper
T. Gundersen and **L. Naess** 503 The synthesis of cost optimal heat exchanger networks—an industrial review of the state of the art

C. A. Floudas and **G. E. Paules IV** 531 A mixed-integer nonlinear programming formulation for the synthesis of heat-integrated distillation sequences

B. Drozdowicz and **E. Martínez** 547 Reduced models for separation processes in real-time simulators

T. O. Odi and **I. A. Karimi** 561 Sizing of intermediate storage for variabilities in noncontinuous processes with parallel units

P. L. Lee and **G. R. Sullivan** 573 Generic model control (GMC)

Zhou Li, Han Zhenwei and **Yu Kuotsung** 581 A new strategy of net decomposition in process simulation

G. Lantagne, B. Marcos and **B. Cayrol** 589 Computation of complex equilibria by nonlinear optimization

Short Note
Y. W. Huang and **L. T. Fan** 601 Fuzzy logic rule based system for separation sequence synthesis: an object-oriented approach

T. L. Wayburn and **J. D. Seader** 609 Letter to the Editor

J. J. Vazquez-Esparragoza, B. McLaughlin, N. W. Naugle and **C. D. Holland** 609 Reply to the Editor

NUMBER 7

ROGER W. H. SARGENT: SPECIAL ISSUE ON PROCESS SYSTEMS ENGINEERING

Gerry Sullivan and **John Perkins** v From the Editors

Roger W. H. Sargent vii Critique

J. B. Hillenbrand Jr and **A. W. Westerberg** 611 The synthesis of multiple-effect evaporator systems using minimum utility insights—I. A cascaded heat representation

A. W. Westerberg and **J. B. Hillenbrand Jr** 625 The synthesis of multiple-effect evaporator systems using minimum utility insights—II. Liquid flow-pattern selection

P. J. Galloway and **B. R. Holt** 637 Multivariable time delay approximations for analysis and control

J. Calandranis and **G. Stephanopoulos** 651 A structural approach to the design of control systems in heat exchanger networks

A. Kretsovalis and **R. S. H. Mah** 671 Observability and redundancy classification in generalized process networks—I. Theorems

A. Kretsovalis and **R. S. H. Mah** 689 Observability and redundancy classification in generalized process networks—II. Algorithms

I. T. Cameron and **R. Gani** 705 Adaptive Runge–Kutta algorithms for dynamic simulation

E. N. Pistikopoulos and **I. E. Grossmann** 719 Optimal retrofit design for improving process flexibility in linear systems

B. E. Ydstie, A. H. Kemna and **L. K. Liu** 733 Multivariable extended-horizon adaptive control

C. C. Pantelides 745 SpeedUp—recent advances in process simulation

E. Zafiriou and **M. Morari** 757 A general controller synthesis methodology based on the IMC structure and the H_2-, H_∞- and μ-optimal control theories

I Softstrip® data strip containing the table of contents of this issue

NUMBER 8

i Softstrip® data strip containing the table of contents of this issue

J. R. Paloschi and **J. D. Perkins** 767 An implementation of quasi-Newton methods for solving sets of nonlinear equations

F. F. Y. Walraven and **P. V. Van Rompay** 777 An improved phase-splitting algorithm

E. Ranzi, M. Rovaglio, T. Faravelli and **G. Biardi** 783 Role of energy balances in dynamic simulation of multicomponent distillation columns

S. S. E. H. Elnashaie and **M. N. Abdel-Hakim** 787 Optimal feed temperature control for fixed bed catalytic reactors experiencing catalyst deactivation—a heterogeneous model

I. D. L. Bogle and **J. D. Perkins** 791 Sparse Newton-like methods in equation oriented flowsheeting

H. Leone, N. Scenna and **A. Vecchietti** 807 An *iso*-propanol distillery revamping using a SIMBAD simulator

J. C. Pinto and **E. C. Biscaia Jr** 821 Order reduction strategies for models of staged separation systems

K. Alejski, J. Szymanowski and **M. Bogacki** 833 The application of a minimization method for solving reacting-distillation problems

E. N. Pistikopoulos and **I. E. Grossmann** 841 Evaluation and redesign for improving flexibility in linear systems with infeasible nominal conditions

E. M. Jongenelen, C. den Heijer and **G. A. van Zee** 845 Detection of gross errors in process data using studentized residuals

Short Note

E. T. Sun and **M. A. Stadtherr** 849 On sparse finite-difference schemes applied to chemical process engineering problems

J. R. Flower 852 Letter to the Editor

NUMBER 9/10

ARTIFICIAL INTELLIGENCE IN CHEMICAL ENGINEERING—RESEARCH AND DEVELOPMENT

Geo. Stephanopoulos and **M. Mavrovouniotis** v Preface

Modeling and Analysis

D. T. Dalle Molle, B. J. Kuipers and **T. F. Edgar** 853 Qualitative modeling and simulation of dynamic systems

M. L. Mavrovouniotis and **G. Stephanopoulos** 867 Formal order-of-magnitude reasoning in process engineering

J. C. Hoskins and **D. M. Himmelblau** 881 Artificial neural network models of knowledge representation in chemical engineering

Diagnosis

T. S. Ramesh, S. K. Shum and **J. F. Davis** 891 A structured framework for efficient problem solving in diagnostic expert systems

V. Venkatasubramanian and **S. H. Rich** 903 An object-oriented two-tier architecture for integrating compiled and deep-level knowledge for process diagnosis

Design

R. Bañares-Alcántara, E. I. Ko, A. W. Westerberg and **M. D. Rychener** 923 DECADE—a hybrid expert system for catalyst selection—II. Final architecture and results

L. Beltramini and **R. L. Motard** 939 KNOD—a knowledge based approach for process design

D. R. Myers, J. F. Davis and **D. J. Herman** 959 A task-oriented approach to knowledge-based systems for process engineering design

Y. W. Huang and **L. T. Fan** 973 Designing an object–relation hybrid database for chemical process engineering

Planning

R. Lakshmanan and **G. Stephanopoulos** 985 Synthesis of operating procedures for complete chemical plants—I. Hierarchical, structured modelling for nonlinear planning

R. Lakshmanan and **G. Stephanopoulos** 1003 Synthesis of operating procedures for complete chemical plants—II. A nonlinear planning methodology

R. H. Fusillo and **G. J. Powers** 1023 Operating procedure synthesis using local models and distributed goals

N. R. Foulkes, M. J. Walton, P. K. Andow and **M. Galluzzo** 1035 Computer-aided synthesis of complex pump and valve operations

Control

G. J. Birky, T. J. McAvoy and **M. Modarres** 1045 An expert system for distillation control design

V. K. Tzouanas, C. Georgakis, W. L. Luyben and **L. H. Ungar** 1065 Expert multivariable control

I Softstrip® data strip containing the table of contents of this issue

NUMBER 11

i Softstrip® data strip containing the table of contents of this issue

M. M. L. Guimarães and **J. J. C. Cruz-Pinto** 1075 Mass transfer and dispersed phase mixing in liquid–liquid systems—I

O. T. Hanna 1083 New explicit and implicit "improved Euler" methods for the integration of ordinary differential equations

S. Vasantharajan and **L. T. Biegler** 1087 Large-scale decomposition for successive quadratic programming

P. E. Arce, A. E. Cassano and **H. A. Irazoqui** 1103 The tubular reactor with laminar flow regime: an integral equation approach—I. Homogeneous reaction with arbitrary kinetics

D. Butala, K. Y. Choi and **M. K. H. Fan** 1115 Multiobjective dynamic optimization of a semi-batch free-radical copolymerization process with interactive CAD tools

E. T. Sun and **M. A. Stadtherr** 1129 Issues in nonlinear equation solving in chemical engineering

F. Duprat, R. Gassend and **G. Gau** 1141 Reactive distillation process optimization by empirical formulae construction

K. Ehrhardt, K. Klusáček and **P. Schneider** 1151 Finite-difference scheme for solving dynamic multicomponent diffusion problems

K. Schnitzlein and **H. Hofmann** 1157 Solving the pellet problem for multicomponent mass transport and complex reactions

R. Y. Qassim and **C. S. Silveira** 1163 Heat exchanger network synthesis: the goal programming approach

Short Note
J. J. Vazquez-Esparragoza, B. E. McLaughlin, N. W. Naugle and **C. D. Holland** 1167 Solution of difficult distillation problems by use of a combination of the Newton–Raphson and functional transformation methods

NUMBER 12

i Softstrip® data strip containing the table of contents of this issue

S. E. Zitney and **M. A. Stadtherr** 1171 Computational experiments in equation-based chemical process flowsheeting

D. R. Lewin and **M. Morari** 1187 ROBEX: an expert system for robust control synthesis

P. B. Gadkari and **R. Govind** 1199 Analytical screening criterion for sequencing of distillation columns

E. N. Pistikopoulos and **I. E. Grossmann** 1215 Stochastic optimization of flexibility in retrofit design of linear systems

M. F. Powers, D. J. Vickery, A. Arehole and **R. Taylor** 1229 A nonequilibrium stage model of multicomponent separation processes—V. Computational methods for solving the model equations

Y. A. Chang and **J. D. Seader** 1243 Simulation of continuous reactive distillation by a homotopy-continuation method

D. L. Miller 1257 Interactive process control panel (a direct manipulation interface for process simulations)

Short Note
A. Lucia and **A. Kumar** 1263 Distillation optimization